

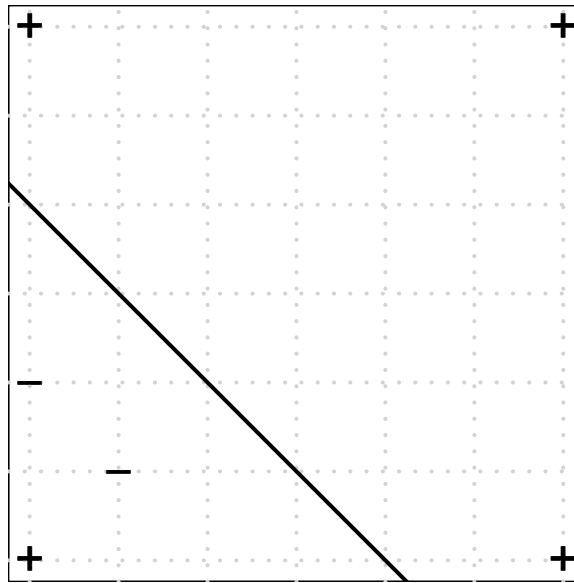
Solution 1: Soft Margin Classifier

(a) The hyperplane is given by:

$$\theta_1 x_1^{(i)} + \theta_2 x_2^{(i)} + \theta_0 = 0 \quad (1)$$

Plugging in the values for the θ s and solving for x_2 , we get the decision boundary as function of x_1 :

$$x_2 = -x_1 + 2 \quad (2)$$

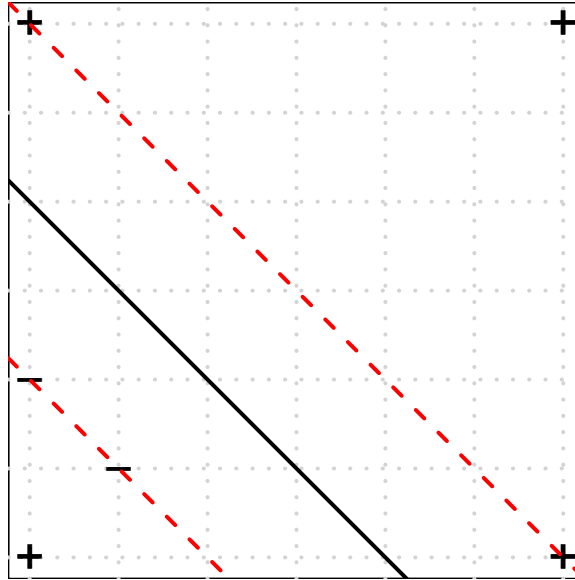


(b) To determine which points are on the margin hyperplanes, we will use the constraint:

$$y^{(i)} (x^{(i)} \hat{\theta} + \hat{\theta}_0) \geq 1 - \zeta^{(i)} \quad (3)$$

$$\left\{ \begin{array}{l} (0, 0) : 1(0 + 0 - 2) = -2 \geq 1 - \zeta^{(1)} \longrightarrow \zeta^{(1)} \geq 3 \\ (0.5, 0.5) : -1(0.5 + 0.5 - 2) = 1 \geq 1 - \zeta^{(2)} \longrightarrow \zeta^{(2)} \geq 0 \\ (0, 1) : -1(0 + 1 - 2) = 1 \geq 1 - \zeta^{(3)} \longrightarrow \zeta^{(3)} \geq 0 \\ (0, 3) : 1(0 + 3 - 2) = 1 \geq 1 - \zeta^{(4)} \longrightarrow \zeta^{(4)} \geq 0 \\ (3, 0) : 1(3 + 0 - 2) = 1 \geq 1 - \zeta^{(5)} \longrightarrow \zeta^{(5)} \geq 0 \\ (3, 3) : 1(3 + 3 - 2) = 4 \geq 1 - \zeta^{(6)} \longrightarrow \zeta^{(6)} \geq -3 \end{array} \right. \quad (4)$$

$(0.5, 0.5), (0, 1), (0, 3), (3, 0)$ lie on the margin hyperplanes $\zeta^{(i)} = 0$.



(c) Using $\mathbf{x}^{(i)} = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$:

$$d(f, \mathbf{x}^{(i)}) = \frac{y^{(i)} f(\mathbf{x}^{(i)})}{\|\theta\|_2} = \frac{-1(0.5 + 0.5 - 2)}{\sqrt{2}} = \frac{1}{\sqrt{2}}$$

The distance is the same for all non-margin-violating support vectors.

(d) Note that $(0, 0)$ is a support vector with slack value of $\zeta^{(i)} = 3$. Some alternatives are:

- Convert the $(0, 0)$ into a negative class.
- Move the $(0, 0)$ to $(2, 2)$.
- Delete $(0, 0)$.

Solution 2: Optimization

- Implementation of the PEGASOS algorithm:

```
#' @param y outcome vector
#' @param X design matrix (including a column of 1s for the intercept)
#' @param nr_iter number of iterations for the algorithm
#' @param theta starting values for thetas
#' @param lambda penalty parameter
#' @param alpha step size for weight decay
pegasos_linear <- function(
  y,
  X,
  nr_iter = 50000,
  theta = rnorm(ncol(X)),
  lambda = 1,
  alpha = 0.01)
{
  t <- 1
  n <- NROW(y)

  while(t <= nr_iter){
```

```

f_current = X%%theta
i <- sample(1:n, 1)

# update
theta <- (1 - lambda * alpha) * theta
# add second term if within margin
if(y[i]*f_current[i] < 1) theta <- theta + alpha * y[i]*X[i,]

t <- t + 1

}

return(theta)

}

```

- Check on a simple example

```

## Check on a simple example
## -----

set.seed(2L)

C = 1

library(mlbench)
library(kernlab)
data = mlbench.twonorm(n = 100, d = 2)

data = as.data.frame(data)
X = as.matrix(data[, 1:2])
y = data$classes
par(mar = c(5,4,4,6))
plot(x = data$x.1, y = data$x.2, pch = ifelse(data$classes == 1, "-", "+"), col = "black",
      xlab = "x1", ylab = "x2")

# recode y
y = ifelse(y == "2", 1, -1)
mod_pegasos = pegasos_linear(y, cbind(1,X), lambda = 1/(C*NROW(y)))

# Add estimated decision boundary:
abline(a = - mod_pegasos[1] / mod_pegasos[3],
       b = - mod_pegasos[2] / mod_pegasos[3], col = "#D55E00")

# Compare to logistic regression:
mod_logreg = glm(classes ~ ., data = data, family = binomial())
abline(a = - coef(mod_logreg)[1] / coef(mod_logreg)[3],
       b = - coef(mod_logreg)[2] / coef(mod_logreg)[3], col = "#56B4E9",
       lty = 3, lwd = 2)

# decision values
f_pegasos = cbind(1,X) %*% mod_pegasos

# How many wrong classified examples?
table(sign(f_pegasos * y))

##

```

```

## -1 1
## 5 95

## compare to kernlab. we CANNOT expect a PERFECT match
## -----

mod_kernlab = ksvm(classes~.,
  data = data,
  kernel = "vanilladot",
  C = C,
  kpar = list(),
  scaled = FALSE)
f_kernlab = predict(mod_kernlab, newdata = data, type = "decision")
# How many wrong classified examples?
table(sign(f_kernlab * y))

##
## -1 1
## 5 95

# compare outputs
print(range(abs(f_kernlab - f_pegasos)))

## [1] 0.00014996 0.38049736

# compare coeffs
# (b is negative offset)
all_params = rbind(
  mod_pegasos,
  mod_kernlab = c(-mod_kernlab@b,
    (params <- colSums(X[mod_kernlab@SVindex, ] *
      mod_kernlab@alpha[[1]] *
      y[mod_kernlab@SVindex])))
)
all_params

##
## mod_pegasos -0.05743352 -1.347267 -0.7917586
## mod_kernlab -0.09763532 -1.263707 -0.7747026

# seems we were reasonably close

# compare empirical risks
emp_risk <- function(theta){
  f = cbind(1, X) %*% theta
  return(0.5 * sum(theta[2:3]^2) + C*sum(ifelse(f > 0, f, 0)))
}
apply(all_params, 1, emp_risk)

## mod_pegasos mod_kernlab
## 153.3287 143.8169

params = all_params[2,]
# recompute margin
margin = 1 / sqrt(sum(params[2:3]^2))

# compute value of intercept shift (the margin shift is in orthogonal direction
# to the decision boundary, so this has to be transformed first)

```

```

m = - params[2] / params[3]
t_0 = margin / (cos(atan(m)))

# add margins to visualization:
#
abline(a = -params[1] / params[3],
       b = m, col = "#0072B2")
abline(a = -params[1] / params[3] + t_0,
       b = m, col = "#0072B2", lty = 2)
abline(a = -params[1] / params[3] - t_0,
       b = m, col = "#0072B2", lty = 2)

# find support vectors on decision border
nv_sv_idx = y[mod_kernlab@SVindex] * f_kernlab[mod_kernlab@SVindex] > 0.98
points(X[mod_kernlab@SVindex[nv_sv_idx],])

# add legends
legend(par('usr')[2], par('usr')[4], , bty='n', xpd=NA, legend=c("1","2"),
       pch=c("-", "+"), title="Classes", cex = 0.8)
legend(par('usr')[2], 1.8, , bty='n', xpd=NA,
       legend=c("Pegasos", "Logistic", "Kernlab", "Margin"),
       lty=c(1,3,1,2),
       col = c("#D55E00", "#56B4E9", "#0072B2", "#0072B2"),
       title="", cex = 0.8, lwd = c(1,2,1,1))

```

